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# Pyridine Derived N-Heterocyclic Carbene Complexes of Platinum: Synthesis, Structure and Ligand Substitution Kinetics

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*Received xxxx xx, 2003*

**Supporting Information Available:** Erying plots and kobs vs. DMSO plots for **1c-4c** and **6**. Crystallographic data and pictures of structures for **1b, 2c-4c, 5** and **6**. (22 pages).

**Figure S1**

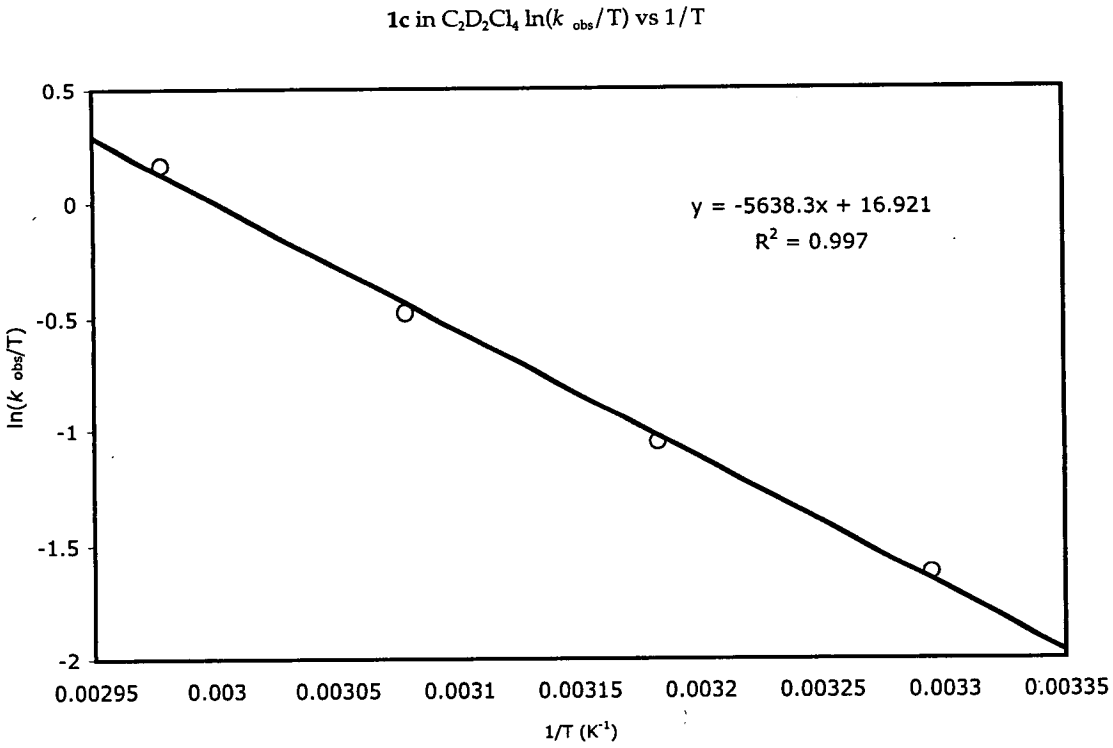



**Figure S2**

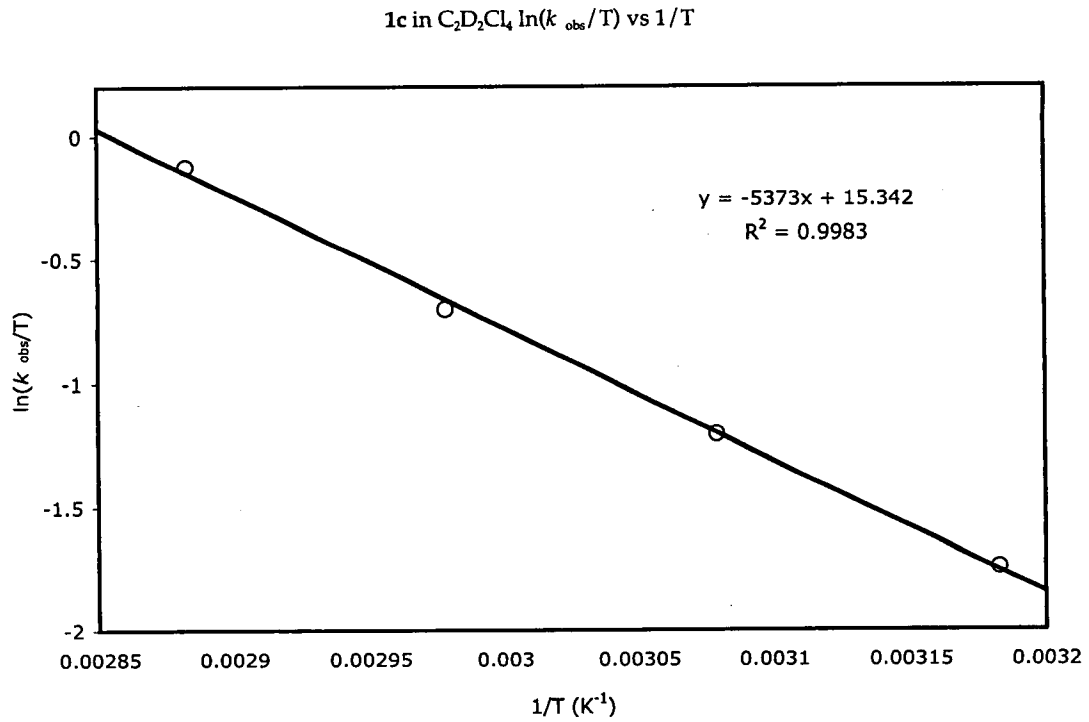


**Figure S3.**

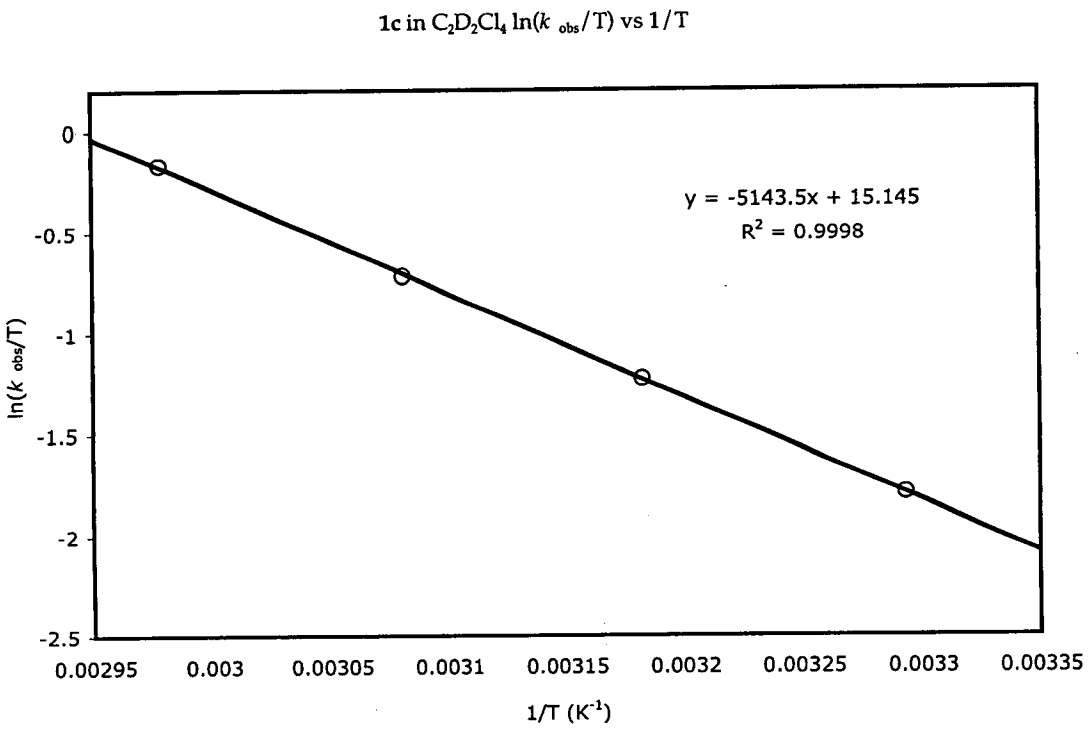
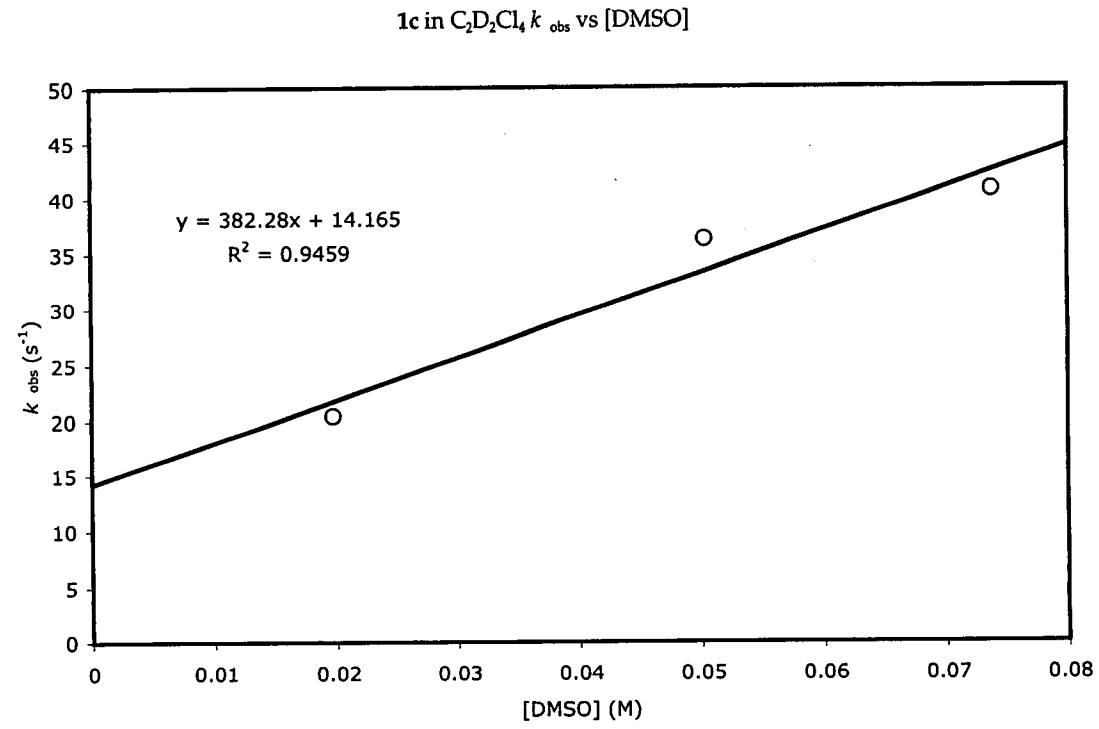



**Figure S4.**



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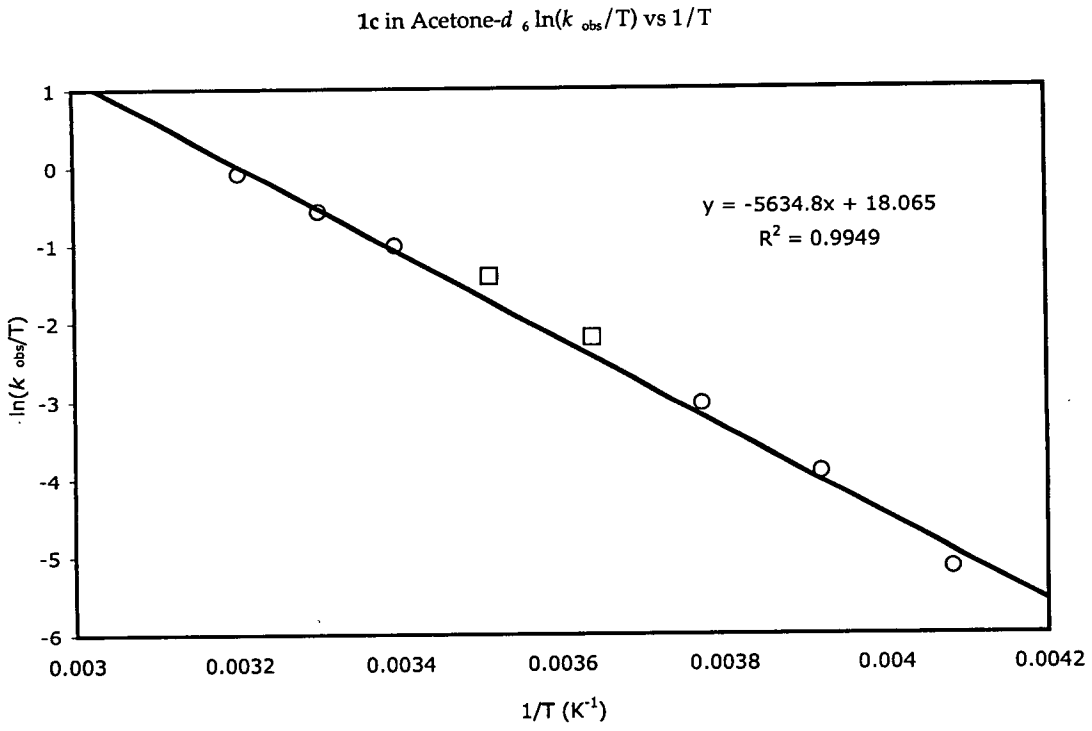
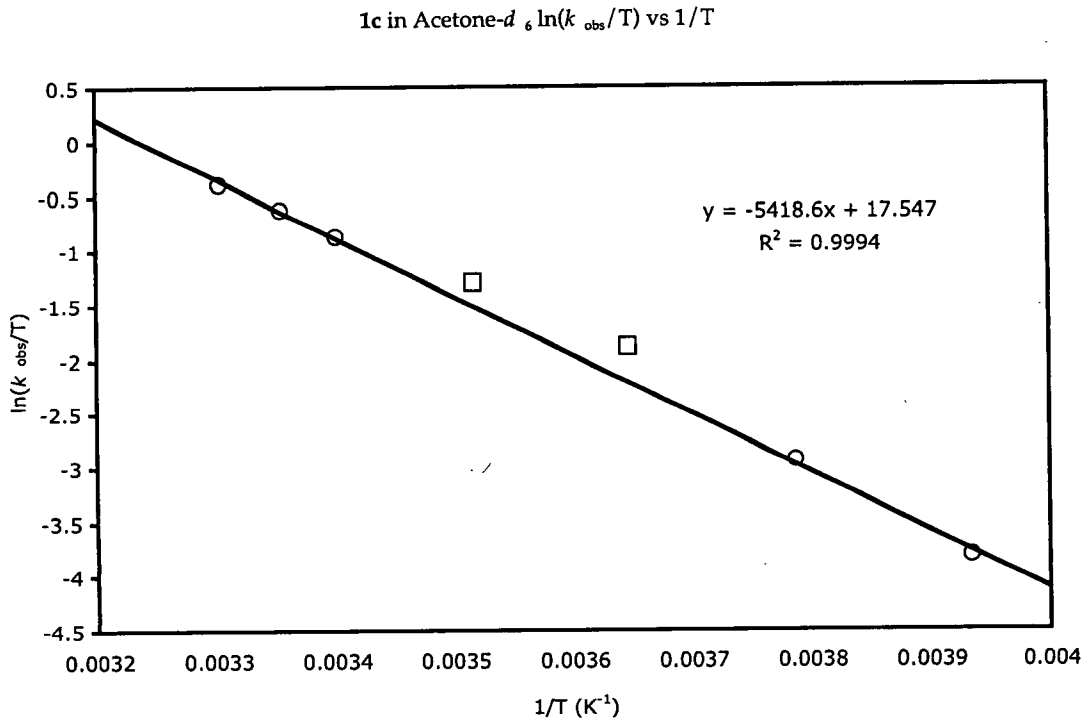



**Figure S6.**



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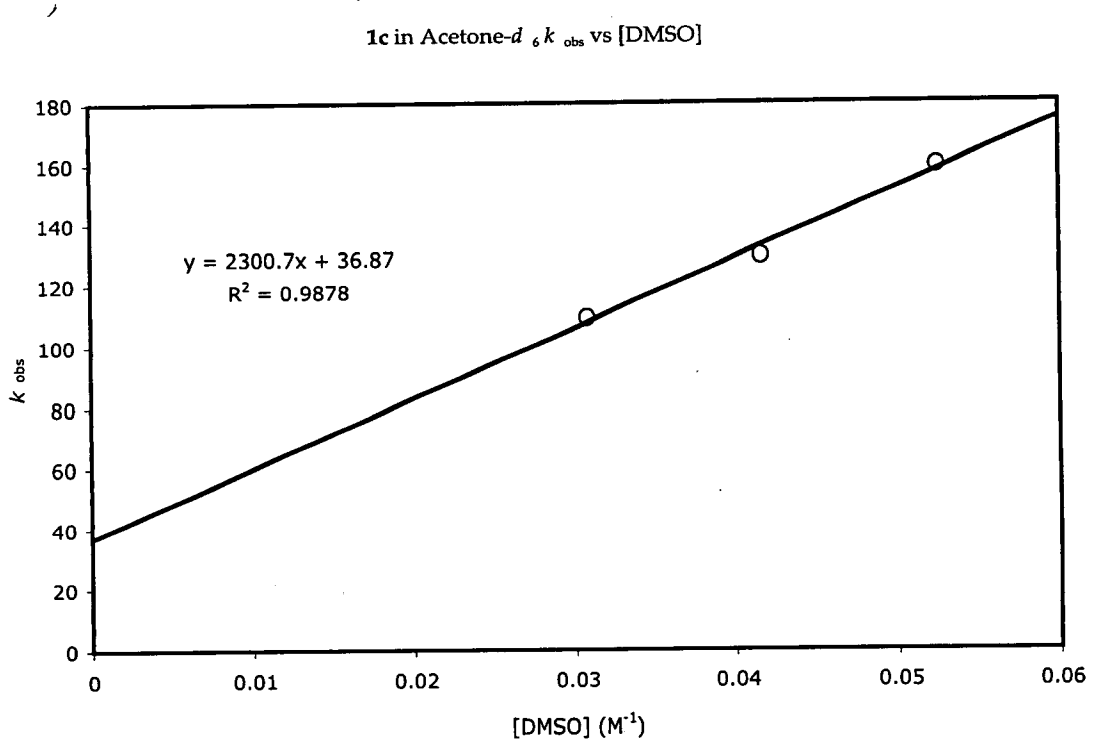



**Figure S8.**

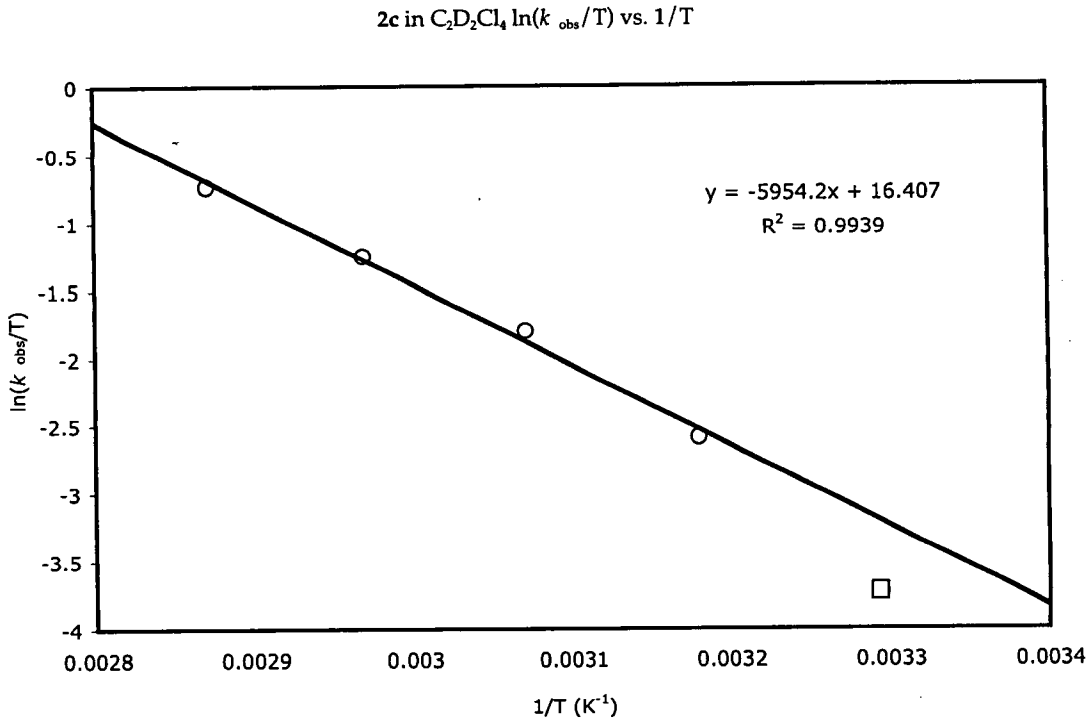
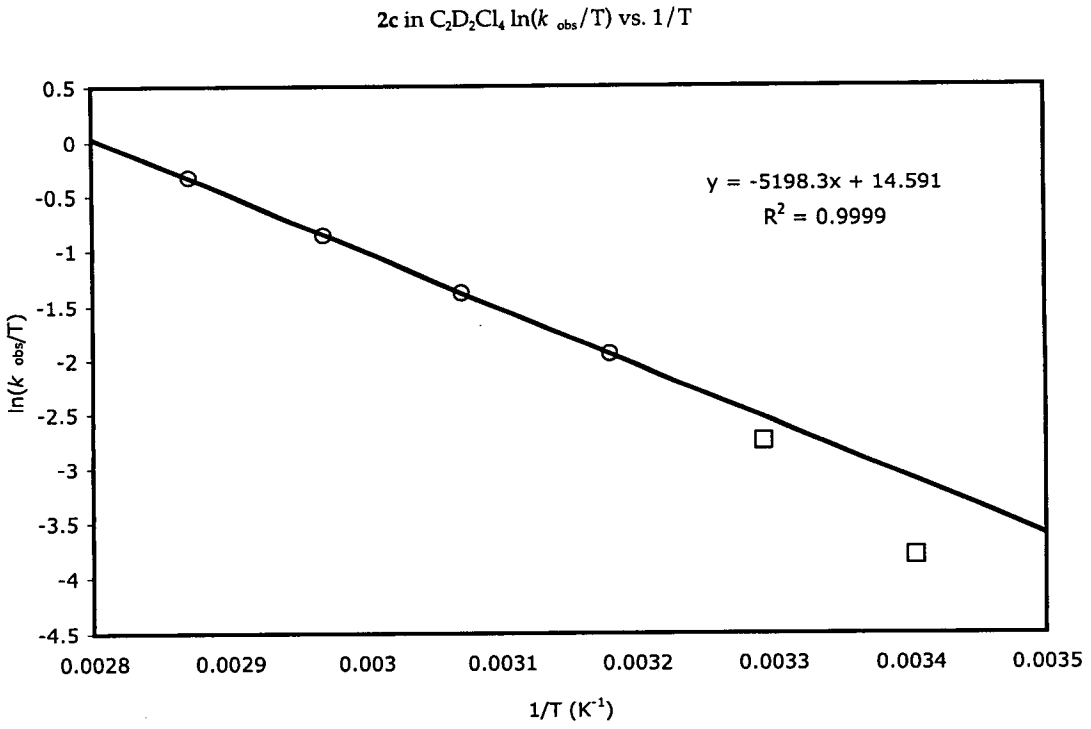


**Figure S9.**

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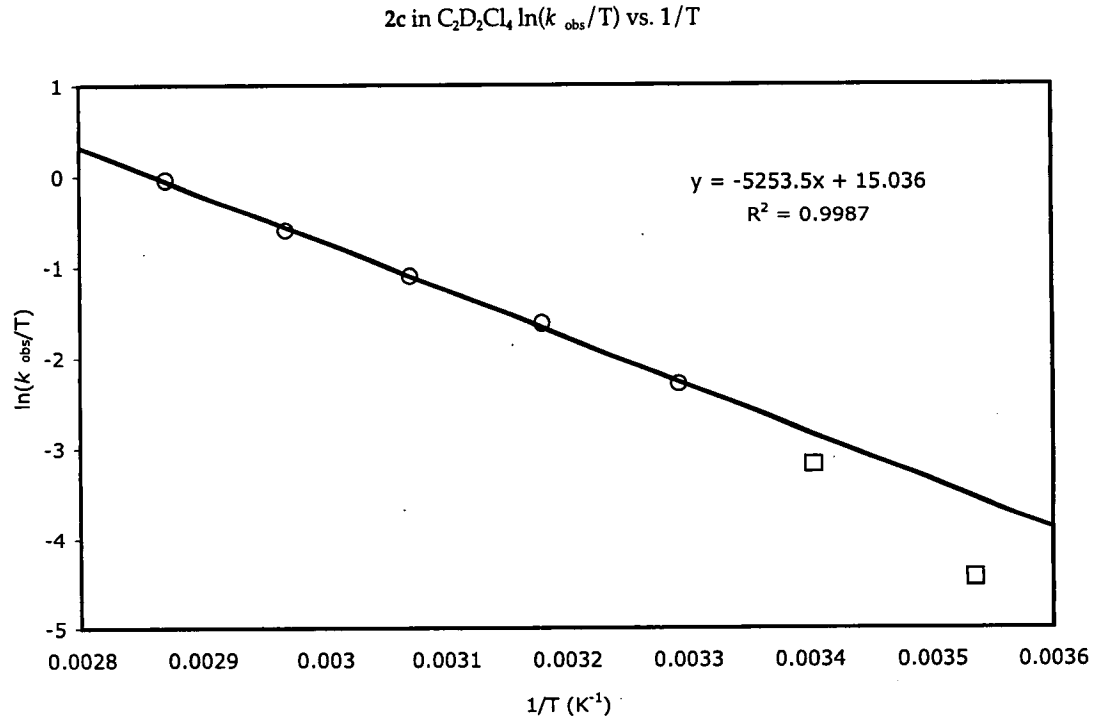


**Figure S11.**

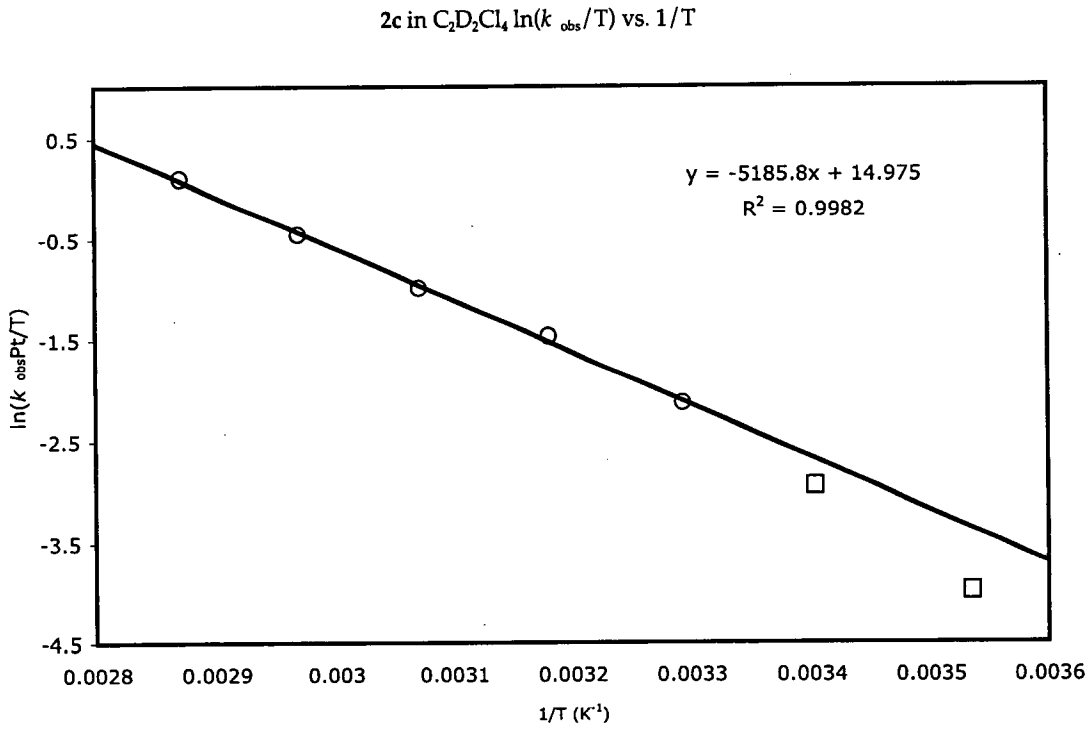
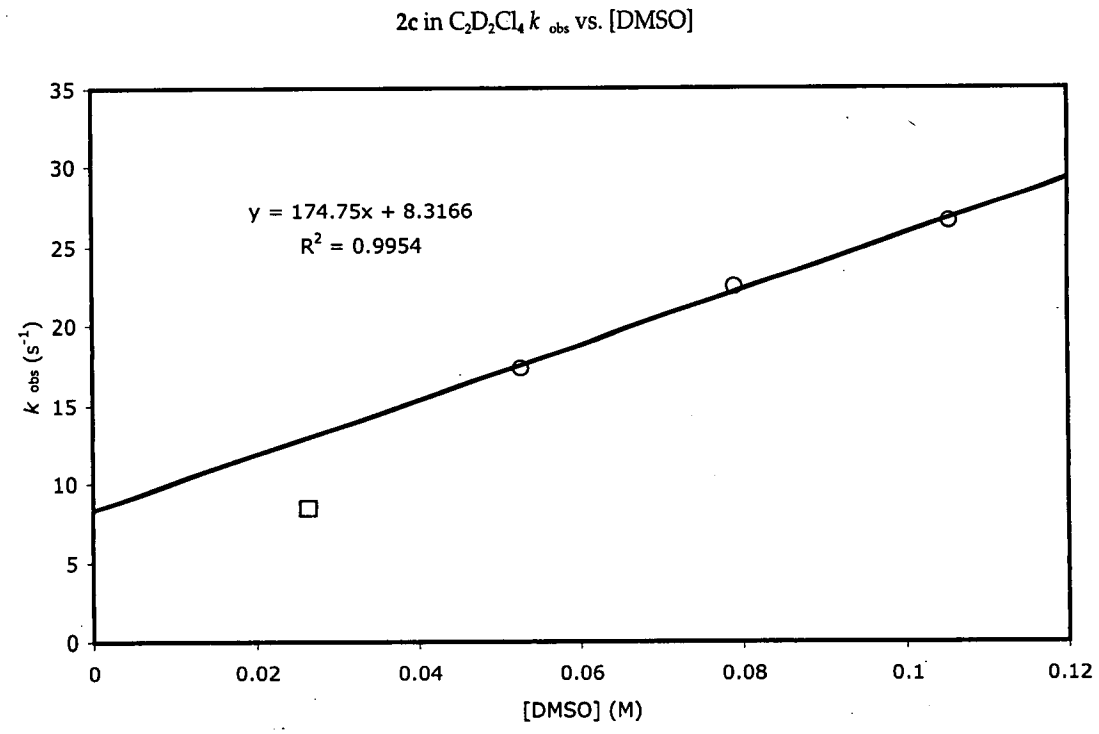



**Figure S12.**



**A note about the effect of 195Pt satellites on the variable temperature 1H-NMR spectra of 1c and 2c.**

195Pt satellites obscure the signals for the platinum bound DMSO and exhibit variable behavior that adds error to the measurement of the linewidth at half height. Spectra with significant, contributions from the satellites at half height are signified by a □ in figures S1-S11 as well as Figure 6 of the main text. These points were ignored when calculating $k_{obs}^{298}$ and activation parameters. Nonetheless these points are shown for completeness.

**Figure S13.**

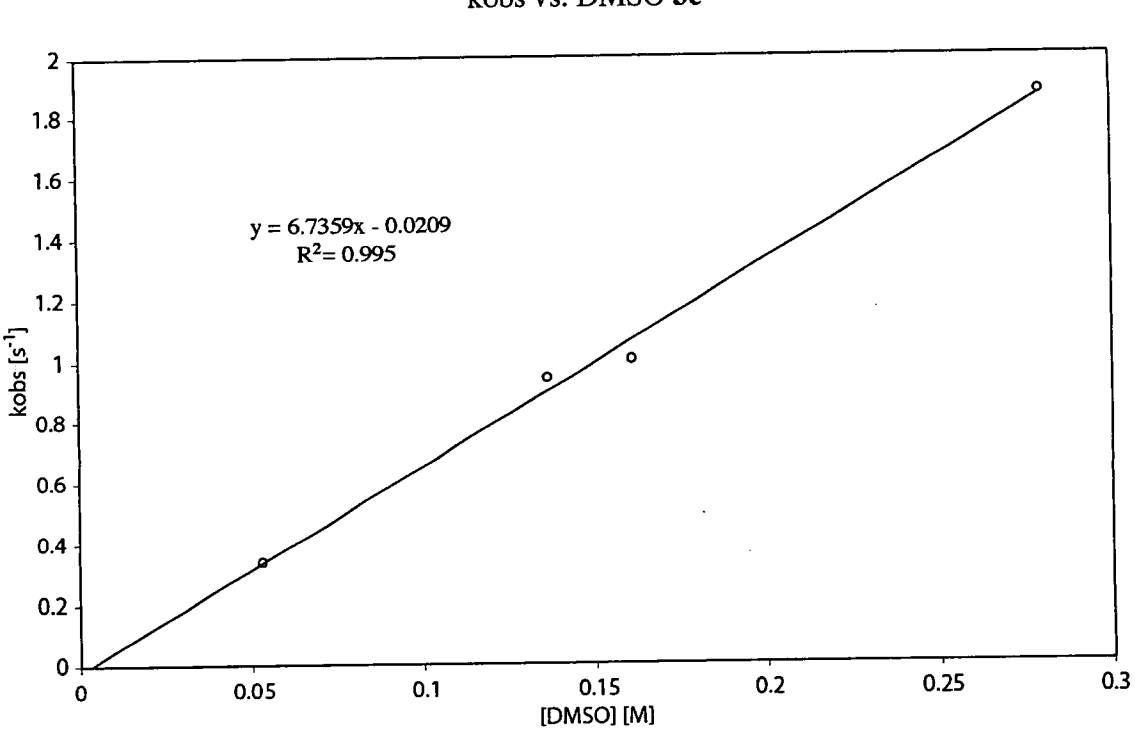



**Figure S14.**

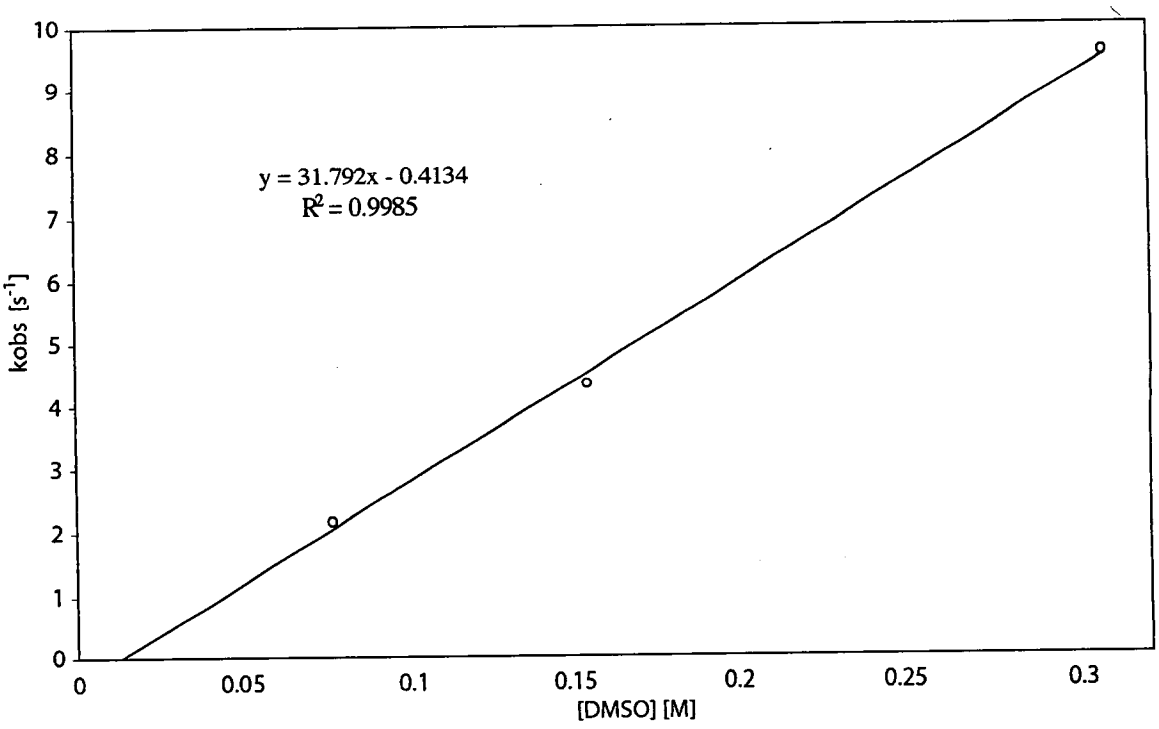
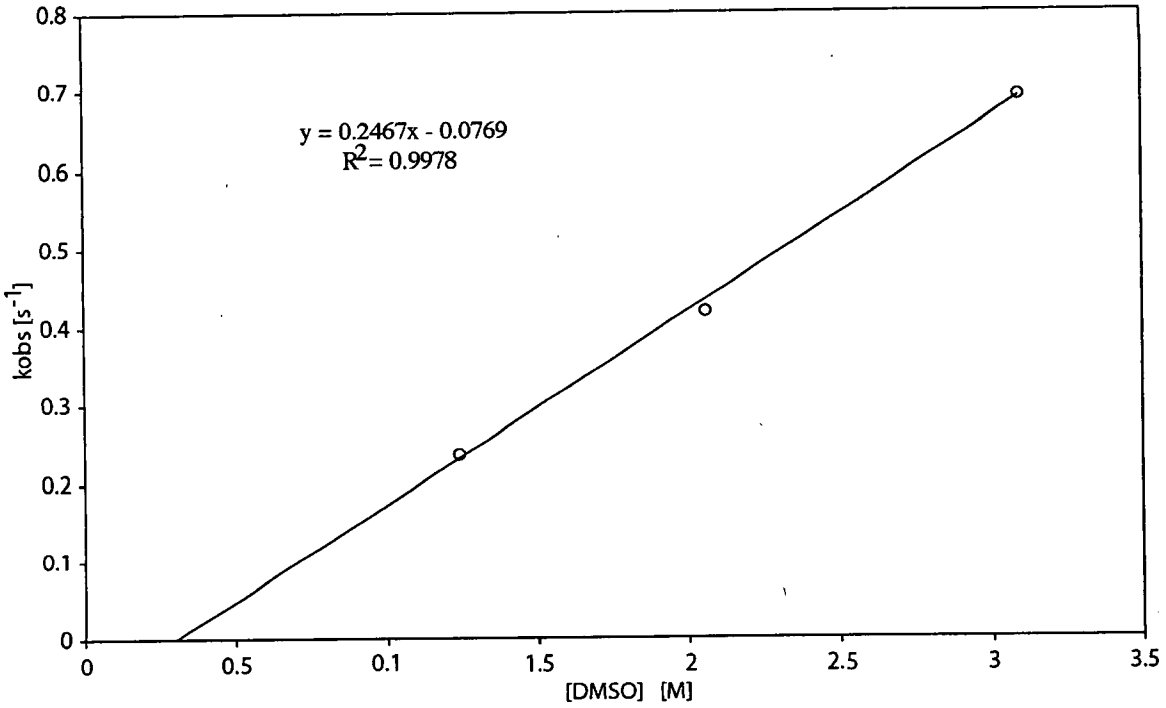


**Figure S15.**

kobs vs [DMSO] for **6**



## Summary of x-ray crystallographic data for complexes 1b, 2c-4c, 5, and 6.

### Table S1. Crystal data and structure refinement for 1b (CCDC 196586).

| | |
|---|---|
| Empirical formula | $[C_{13}H_{17}N_2SPt]^+[B(C_6H_5)_4]^- \cdot C_3H_6O$ |
| Formula weight | 805.72 |
| Crystallization Solvent | Acetone |
| Crystal Habit | Prism |
| Crystal size | 0.21 x 0.12 x 0.11 $mm^3$ |
| Crystal color | Yellow |

### Data Collection

| | | |
|---|---|---|
| Preliminary Photos | Rotation | |
| Type of diffractometer | Bruker SMART 1000 | |
| Wavelength | 0.71073 Å MoKα | |
| Data Collection Temperature | 98(2) K | |
| θ range for 23028 reflections used in lattice determination | 2.29 to 28.22° | |
| Unit cell dimensions | a = 11.0611(6) Å | α= 114.0150(10)° |
| | b = 13.0966(7) Å | β= 91.9270(10)° |
| | c = 14.2868(7) Å | γ = 111.0610(10)° |
| Volume | 1724.46(16) $Å^3$ | |
| Z | 2 | |
| Crystal system | Triclinic | |
| Space group | P-1 | |
| Density (calculated) | 1.552 $Mg/m^3$ | |
| F(000) | 808 | |
| Data collection program | Bruker SMART v5.054 | |
| θ range for data collection | 1.60 to 28.30° | |
| Completeness to θ = 28.30° | 91.7 % | |
| Index ranges | $-14 \le h \le 14, -17 \le k \le 17, -18 \le l \le 18$ | |
| Data collection scan type | ω scans at 7 ϕ settings | |
| Data reduction program | Bruker SAINT v6.022 | |
| Reflections collected | 35217 | |
| Independent reflections | 7878 [$R_{int}$= 0.0743] | |
| Absorption coefficient | 4.163 $mm^{-1}$ | |
| Absorption correction | None | |
| Max. and min. transmission | 0.6574 and 0.4751 | |

### Structure solution and Refinement

| | |
|---|---|
| Structure solution program | SHELXS-97 (Sheldrick, 1990) |
| Primary solution method | Patterson method |
| Secondary solution method | Difference Fourier map |
| Hydrogen placement | Difference Fourier map |
| Structure refinement program | SHELXL-97 (Sheldrick, 1997) |
| Refinement method | Full matrix least-squares on $F^2$ |
| Data / restraints / parameters | 7878 / 0 / 587 |
| Treatment of hydrogen atoms | Unrestrained |
| Goodness-of-fit on $F^2$ | 1.215 |
| Final R indices [I>2σ(I), 7050 reflections] | R1 = 0.0244, *w*R2 = 0.0509 |
| R indices (all data) | R1 = 0.0290, *w*R2 = 0.0517 |
| Type of weighting scheme used | Sigma |
| Weighting scheme used | $w=1/\sigma^2(Fo^2)$ |
| Max shift/error | 0.002 |
| Average shift/error | 0.000 |

**Table S1 (cont.)**

| | |
|---|---|
| Largest diff. peak and hole | 1.781 and -0.931 e.Å$^{-3}$ |

## Special Refinement Details

All peaks in the final electron density Fourier maps greater than one electron lie within an angstrom of the platinum atom. Acetone is included in the crystals as a solvent of crystallization. The position of the acetone molecule is well defined and is incorporated in the model. No restraints were applied during least-squares refinement.

Refinement of $F^2$ against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on $F^2$, conventional R-factors (R) are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2s(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

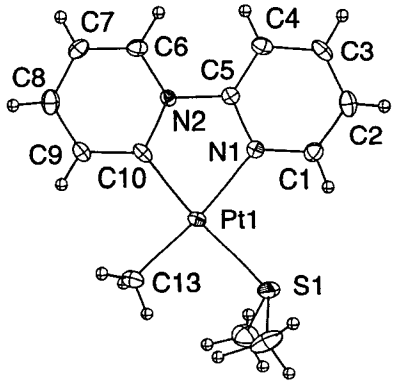


**Table S2. Crystal data and structure refinement for 2c (CCDC 187696).**

| | |
|---|---|
| Empirical formula | $[C_{17}H_{22}N_2OSPt]^+[SO_3CF_3]^- \cdot \_(C_6H_6)$ |
| Formula weight | 685.64 |
| Crystallization Solvent | Acetone/benzene |
| Crystal Habit | Plate |
| Crystal size | 0.23 x 0.10 x 0.04 $mm^3$ |
| Crystal color | Pale yellow |

## Data Collection

| | |
|---|---|
| Preliminary Photos | Rotation |
| Type of diffractometer | Bruker SMART 1000 |
| Wavelength | 0.71073 Å MoKα |
| Data Collection Temperature | 98(2) K |
| θ range for 20473 reflections used in lattice determination | 2.16 to 27.88° |
| Unit cell dimensions | a = 21.8153(11) Å<br>b = 10.4419(5) Å<br>c = 22.0778(11) Å |
| Volume | 5029.2(4) $Å^3$ |
| Z | 8 |
| Crystal system | Orthorhombic |
| Space group | Pbcn |
| Density (calculated) | 1.811 $Mg/m^3$ |
| F(000) | 2672 |
| θ range for data collection | 1.84 to 28.42° |
| Completeness to θ = 28.42° | 97.5 % |
| Index ranges | $-28 \le h \le 28, -13 \le k \le 13, -28 \le l \le 29$ |
| Data collection scan type | ω scans at 7 ϕ settings |
| Reflections collected | 98949 |
| Independent reflections | 6163 [$R_{int}$= 0.1341] |
| Absorption coefficient | 5.797 $mm^{-1}$ |
| Absorption correction | None |
| Max. and min. transmission | 0.8012 and 0.3490 |

## Structure solution and Refinement

| | |
|---|---|
| Structure solution program | SHELXS-97 (Sheldrick, 1990) |
| Primary solution method | Direct methods |
| Secondary solution method | Difference Fourier map |
| Hydrogen placement | Geometric positions |
| Structure refinement program | SHELXL-97 (Sheldrick, 1997) |
| Refinement method | Full matrix least-squares on $F^2$ |
| Data / restraints / parameters | 6163 / 15 / 324 |
| Treatment of hydrogen atoms | Riding |
| Goodness-of-fit on $F^2$ | 1.860 |
| Final R indices [I>2σ(I), 3593 reflections] | R1 = 0.0496, *w*R2 = 0.0806 |
| R indices (all data) | R1 = 0.1088, *w*R2 = 0.0883 |
| Type of weighting scheme used | Sigma |
| Weighting scheme used | $w=1/\sigma^2(Fo^2)$ |
| Max shift/error | 0.003 |
| Average shift/error | 0.000 |
| Largest diff. peak and hole | 3.235 and -2.575 $e.Å^{-3}$ |

**Table S2 (cont.)**

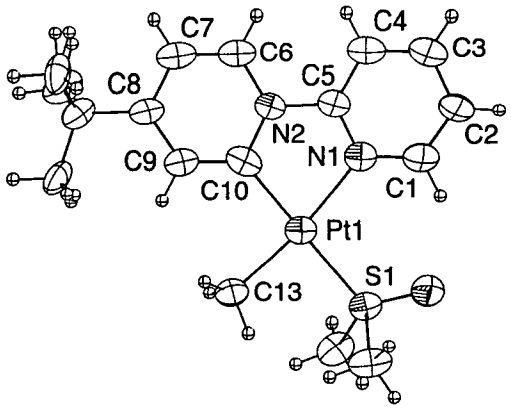
## Special Refinement Details

The tertiary butyl group bonded to C11 is disordered, the methyl carbons are rotated by less than 60° about the C11-C14 bond. The major component (~70%) was modeled with anisotropic displacement parameters and the minor component (~30%) was modeled isotropically. The bonds between the tertiary carbon (C11) and the methyl carbons (of both orientations) were restrained to be equal but allowed to vary in length. No other restraints were placed on the geometry of this group. However, the counter ion required restraints for the distances and angles of the flourine atoms. The crystals contain a molecule of benzene located on a center of symmetry.

No absorption correction was applied to the data. All significant residual electron density in the final difference Fourier map is near platinum or the counterion.

Refinement of $F^2$ against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on $F^2$, conventional R-factors (R) are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.



## Table S3. Crystal data and structure refinement for 3c (CCDC 181466).

| | |
|---|---|
| Empirical formula | $[C_{15}H_{22}BN_3OSPt]^+ [B(C_6H_5)_4]^-$ |
| Formula weight | 806.72 |
| Crystallization Solvent | Dichloromethane/Diethylether |
| Crystal Habit | Block |
| Crystal size | 0.24 x 0.17 x 0.16 $mm^3$ |
| Crystal color | Pale yellow |

## Data Collection

| | |
|---|---|
| Preliminary Photos | Rotation |
| Type of diffractometer | Bruker SMART 1000 |
| Wavelength | 0.71073 Å MoKα |
| Data Collection Temperature | 98(2) K |
| θ range for 27853 reflections used in lattice determination | 2.50 to 28.3° |
| Unit cell dimensions | a = 11.0499(4) Å, α= 67.7790(10)° |
| | b = 11.3835(4) Å, β= 74.5460(10)° |
| | c = 14.9527(6) Å, γ = 88.1200(10)° |
| Volume | 1673.33(11) $Å^3$ |
| Z | 2 |
| Crystal system | Triclinic |
| Space group | P-1 |
| Density (calculated) | 1.601 $Mg/m^3$ |
| F(000) | 808 |
| Data collection program | Bruker SMART v5.054 |
| θ range for data collection | 1.53 to 28.35° |
| Completeness to θ = 28.35° | 92.2 % |
| Index ranges | $-14 \le h \le 14, -15 \le k \le 15, -19 \le l \le 19$ |
| Data collection scan type | ω scans at 7 ϕ settings |
| Data reduction program | Bruker SAINT v6.022 |
| Reflections collected | 34531 |
| Independent reflections | 7711 [$R_{int}$= 0.0709] |
| Absorption coefficient | 4.291 $mm^{-1}$ |
| Absorption correction | None |
| Max. and min. transmission | 0.5468 and 0.4257 |

## Structure solution and Refinement

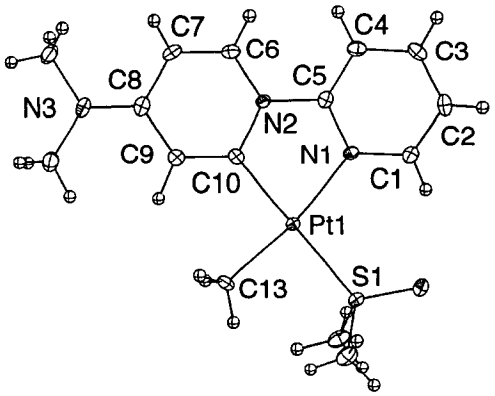
| | |
|---|---|
| Structure solution program | SHELXS-86 (Sheldrick, 1986) |
| Primary solution method | Direct methods |
| Secondary solution method | Difference Fourier map |
| Hydrogen placement | Difference Fourier map |
| Structure refinement program | SHELXL-97 (Sheldrick, 1997) |
| Refinement method | Full matrix least-squares on $F^2$ |
| Data / restraints / parameters | 7711 / 0 / 583 |
| Treatment of hydrogen atoms | Unrestrained |
| Goodness-of-fit on $F^2$ | 1.365 |
| Final R indices [I>2σ(I), 7290 reflections] | R1 = 0.0203, *w*R2 = 0.0470 |
| R indices (all data) | R1 = 0.0220, *w*R2 = 0.0473 |
| Type of weighting scheme used | Sigma |
| Weighting scheme used | $w=1/\sigma^2(Fo^2)$ |
| Max shift/error | 0.003 |
| Average shift/error | 0.000 |
| Largest diff. peak and hole | 1.904 and -1.013 e.$Å^{-3}$ |

**Table S3 (cont.)**

## Special Refinement Details

Refinement of $F^2$ against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on $F^2$, conventional R-factors (R) are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.



## Table S4. Crystal data and structure refinement for 4c (CCDC 198660).

| | |
|---|---|
| Empirical formula | $[C_{15}H_{22}N_3OSPt]^+ [B(C_6H_5)_4]^- \cdot \_(C_3H_6O)$ |
| Formula weight | 835.76 |
| Crystallization Solvent | Acetone/petroleum ether |
| Crystal Habit | Block |
| Crystal size | 0.13 x 0.11 x 0.08 $mm^3$ |
| Crystal color | Red |

### Data Collection

| | |
|---|---|
| Preliminary Photos | Rotation |
| Type of diffractometer | Bruker SMART 1000 |
| Wavelength | 0.71073 Å MoKα |
| Data Collection Temperature | 98(2) K |
| θ range for 22823 reflections used in lattice determination | 2.35 to 28.29° |
| Unit cell dimensions | a = 11.1872(6) Å<br>b = 15.3712(8) Å β= 90.4650(10)°<br>c = 20.8806(10) Å |
| Volume | 3590.5(3) $Å^3$ |
| Z | 4 |
| Crystal system | Monoclinic |
| Space group | $P2_1$ |
| Density (calculated) | 1.546 $Mg/m^3$ |
| F(000) | 1680 |
| Data collection program | Bruker SMART v5.054 |
| θ range for data collection | 1.65 to 28.39° |
| Completeness to θ = 28.39° | 94.2 % |
| Index ranges | $-14 \le h \le 14, -20 \le k \le 20, -27 \le l \le 27$ |
| Data collection scan type | ω scans at 5 ϕ settings |
| Data reduction program | Bruker SAINT v6.022 |
| Reflections collected | 53484 |
| Independent reflections | 16452 [$R_{int}$= 0.0693] |
| Absorption coefficient | 4.004 $mm^{-1}$ |
| Absorption correction | None |
| Max. and min. transmission | 0.7401 and 0.6241 |

### Structure solution and Refinement

| | |
|---|---|
| Structure solution program | SHELXS-97 (Sheldrick, 1990) |
| Primary solution method | Direct methods |
| Secondary solution method | Difference Fourier map |
| Hydrogen placement | Geometric positions |
| Structure refinement program | SHELXL-97 (Sheldrick, 1997) |
| Refinement method | Full matrix least-squares on $F^2$ |
| Data / restraints / parameters | 16452 / 1 / 878 |
| Treatment of hydrogen atoms | Riding |
| Goodness-of-fit on $F^2$ | 1.074 |
| Final R indices [I>2σ(I), 14326 reflections] | R1 = 0.0343, *w*R2 = 0.0601 |
| R indices (all data) | R1 = 0.0442, *w*R2 = 0.0624 |
| Type of weighting scheme used | Sigma |
| Weighting scheme used | $w=1/\sigma^2(Fo^2)$ |
| Max shift/error | 0.010 |
| Average shift/error | 0.000 |
| Absolute structure parameter | 0.600(5) |
| Largest diff. peak and hole | 1.383 and -0.871 e.$Å^{-3}$ |

**Table S4 (cont.)**

## Special Refinement Details

The intensities of the *h0l* reflections are systematically weak when *h+l* is odd compared to when *h+l* is even but the weak reflections are sufficiently strong enough to be considered as observed. This systematic observation of *h0l* reflections indicates the correct choice of space group is non-centrosymmetric $P2_1$ and not centrosymmetric $P2_1/n$. Refinement in the centrosymmetric space group produces many atoms with non-positive definite anisotropic displacement parameters (ADP's) or ADP's with extremely elliptical shapes. When refined in the non-centrosymmetric space group the value of the Flack parameter (twin index) suggests racemic twinning, ratio 60:40. The conclusion is that racemic twinning is present in these crystals. Therefore, twinning was accounted for during refinement using a TWIN card. Each asymmetric unit contains one acetone molecule in addition to two anion-cation pairs. Bond distances and angles for both molecules of the platinum complex in the asymmetric unit agree within 3σ (see Table 3) and the averaged values should be quite reliable.

Refinement of $F^2$ against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on $F^2$, conventional R-factors (R) are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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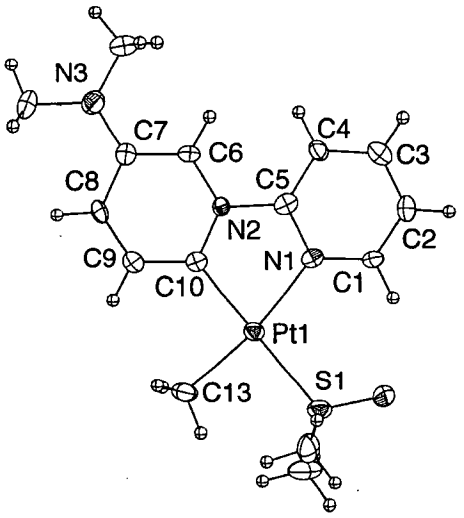


**4c**

**Table S5. Crystal data and structure refinement for 5 (CCDC 196451).**

| | |
|---|---|
| Empirical formula | $[C_{13}H_{17}N_2OPtS]^+[B(C_6H_5)_4]^- \cdot \_(C_3H_6O)$ |
| Formula weight | 792.69 |
| Crystallization Solvent | Acetone/Petroleum ether |
| Crystal Habit | Prism |
| Crystal size | 0.17 x 0.13 x 0.09 $mm^3$ |
| Crystal color | Colorless |

## Data Collection

| | |
|---|---|
| Preliminary Photos | Rotation |
| Type of diffractometer | Bruker SMART 1000 |
| Wavelength | 0.71073 Å MoKα |
| Data Collection Temperature | 98(2) K |
| θ range for 32807 reflections used in lattice determination | 2.24 to 28.38° |
| Unit cell dimensions | a = 23.0688(8) Å<br>b = 13.1532(5) Å β= 115.5560(10)°<br>c = 23.9873(9) Å |
| Volume | 6566.3(4) $Å^3$ |
| Z | 8 |
| Crystal system | Monoclinic |
| Space group | $P2_1/c$ |
| Density (calculated) | 1.604 $Mg/m^3$ |
| F(000) | 3168 |
| θ range for data collection | 1.71 to 28.60° |
| Completeness to θ = 28.60° | 94.7 % |
| Index ranges | $-31 \le h \le 30, -17 \le k \le 17, -31 \le l \le 31$ |
| Data collection scan type | ω scans at 7 ϕ settings |
| Reflections collected | 135233 |
| Independent reflections | 15907 [$R_{int}$= 0.0844] |
| Absorption coefficient | 4.373 $mm^{-1}$ |
| Absorption correction | Face-indexed Gaussian |
| Max. and min. transmission | 0.69397 and 0.56537 |

## Structure solution and Refinement

| | |
|---|---|
| Structure solution program | SHELXS-97 (Sheldrick, 1990) |
| Primary solution method | Direct methods |
| Secondary solution method | Difference Fourier map |
| Hydrogen placement | Geometric positions |
| Structure refinement program | SHELXL-97 (Sheldrick, 1997) |
| Refinement method | Full matrix least-squares on $F^2$ |
| Data / restraints / parameters | 15907 / 0 / 838 |
| Treatment of hydrogen atoms | Riding |
| Goodness-of-fit on $F^2$ | 1.290 |
| Final R indices [I>2σ(I), 10117 reflections] | R1 = 0.0359, *w*R2 = 0.0538 |
| R indices (all data) | R1 = 0.0750, *w*R2 = 0.0578 |
| Type of weighting scheme used | Sigma |
| Weighting scheme used | $w=1/\sigma^2(Fo^2)$ |
| Max shift/error | 0.002 |
| Average shift/error | 0.000 |
| Largest diff. peak and hole | 2.486 and -1.748 $e.Å^{-3}$ |

**Table S5 (cont.)**

## Special Refinement Details

Disorder exists in this crystal. Molecule B appears to occupy two orientations, differing by an approximate 180° rotation about an axis in the plane of the molecule and a displacement along a vector parallel to the plane of the molecule of nearly 1Å (see Figures 2 and 5). The relative populations of these two orientations is approximately 85:15 (see Table 2). No restraints were placed on the atomic positions of the minor component and no attempt was made to model the positions of the remaining atoms for that component. Residual electron density in the final difference Fourier maps greater than one electron are within an angstrom of platinum.

Refinement of $F^2$ against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on $F^2$, conventional R-factors (R) are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

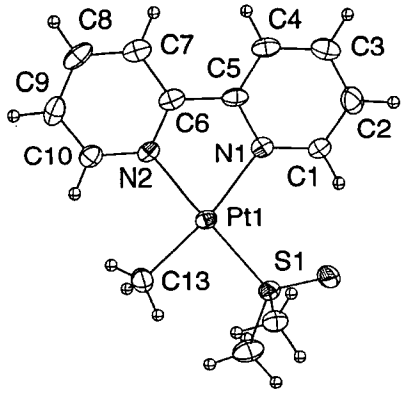

**Table S6. Crystal data and structure refinement for 6 (CCDC 195233).**

| | |
|---|---|
| Empirical formula | $C_{14}H_{17}NOSPt$ |
| Formula weight | 442.44 |
| Crystallization Solvent | Acetone/DSMO |
| Crystal Habit | Prism |
| Crystal size | 0.14 x 0.11 x 0.07 $mm^3$ |
| Crystal color | Yellow |

## Data Collection

| | |
|---|---|
| Preliminary Photos | Rotation |
| Type of diffractometer | Bruker SMART 1000 |
| Wavelength | 0.71073 Å MoKα |
| Data Collection Temperature | 98(2) K |
| θ range for 14557 reflections used in lattice determination | 2.33 to 28.35° |
| Unit cell dimensions | a = 10.3677(9) Å<br>b = 14.9165(13) Å<br>c = 17.3745(15) Å |
| Volume | 2687.0(4) $Å^3$ |
| Z | 8 |
| Crystal system | Orthorhombic |
| Space group | Pbca |
| Density (calculated) | 2.187 $Mg/m^3$ |
| F(000) | 1680 |
| Data collection program | Bruker SMART v5.054 |
| θ range for data collection | 2.34 to 28.49° |
| Completeness to θ = 28.49° | 96.1 % |
| Index ranges | $-13 \le h \le 13$, $-19 \le k \le 19$, $-23 \le l \le 22$ |
| Data collection scan type | ω scans at 5 ϕ settings |
| Data reduction program | Bruker SAINT v6.022 |
| Reflections collected | 37689 |
| Independent reflections | 3270 [$R_{int}$= 0.0694] |
| Absorption coefficient | 10.586 $mm^{-1}$ |
| Absorption correction | Gaussian Face-indexed |
| Max. and min. transmission | 0.5197 and 0.2403 |

## Structure solution and Refinement

| | |
|---|---|
| Structure solution program | SHELXS-97 (Sheldrick, 1990) |
| Primary solution method | Patterson method |
| Secondary solution method | Difference Fourier map |
| Hydrogen placement | Geometric positions |
| Structure refinement program | SHELXL-97 (Sheldrick, 1997) |
| Refinement method | Full matrix least-squares on $F^2$ |
| Data / restraints / parameters | 3270 / 0 / 166 |
| Treatment of hydrogen atoms | Riding |
| Goodness-of-fit on $F^2$ | 1.272 |
| Final R indices [$I>2\sigma(I)$, 2488 reflections] | R1 = 0.0235, *w*R2 = 0.0364 |
| R indices (all data) | R1 = 0.0388, *w*R2 = 0.0381 |
| Type of weighting scheme used | Sigma |
| Weighting scheme used | $w=1/\sigma^2(Fo^2)$ |
| Max shift/error | 0.002 |
| Average shift/error | 0.000 |
| Largest diff. peak and hole | 2.140 and -0.837 $e.Å^{-3}$ |

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**Table S6 (cont.)**

## Special Refinement Details

Data were corrected for absorption using the Gaussian Face-indexed correction feature in XPREP. Peaks in the final difference Fourier map greater than $1e^{-}/Å^3$ are within 1Å of the platinum atom.

Refinement of $F^2$ against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on $F^2$, conventional R-factors (R) are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.